

The Mechanism of Selective Oxidation of Propene to Acrolein on Bismuth Molybdates from Quantum Mechanics Calculations

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Gas Phase Energy, Zero Point Energy, Vibrational Frequencies, and Coordinates for all compounds mentioned in the manuscript:

Propene Activation on Bi₄O₇

1 (C₃H₆)

Gas Phase Energy = -117.913994 hartrees

Zero Point Energy = 50.085 kcal/mol

Vibrational Frequencies (cm⁻¹): 210.80 424.04 588.85 929.83 938.14 949.39
1033.04 1073.76 1195.52 1330.50 1419.65 1460.46 1492.90 1506.95 1732.64
3028.41 3078.29 3115.68 3141.25 3150.89 3234.12

Coordinates:

C1	-.2661681281	.3718022314	.0000000000
C2	.9950838279	.8023433090	.0000000000
H3	1.2371132385	1.8610574289	.0000000000
H4	1.8340412948	.1100174580	.0000000000
C5	-.6916999571	-1.0681113748	.0000000000
H6	.1703165122	-1.7420906026	.0000000000
H7	-1.3061272373	-1.2990650372	-.8796205569
H8	-1.3061272373	-1.2990650372	.8796205569
H9	-1.0723380432	1.1066151458	.0000000000

1 (Bi₄O₇)

Gas Phase Energy = -548.424876 hartrees

Zero Point Energy = 13.448 kcal/mol

Vibrational Frequencies(cm⁻¹): 91.67 91.76 125.91 126.40 129.01 137.99 138.14
139.67 149.21 149.59 209.00 277.73 280.91 281.34 370.70 371.08 391.95
408.29 408.65 448.13 569.30 581.48 582.52 721.16 734.28 745.45 745.84

Coordinates:

Bi1	-2.1417607083	3.1859331469	-0.3249013049
O2	-0.2497022654	2.4852565620	-0.4464660510
O3	-2.0224415784	3.8425058313	1.6049814990
O4	-3.0379654985	1.4232876411	0.0958254652
Bi5	-2.5811774225	-0.0465923406	1.4062240594

O6	-2.3839758719	1.1607538446	3.0422974765
Bi7	-1.3303893719	2.8536783091	3.1985456142
O8	0.4359692996	2.2345603525	2.4928896254
Bi9	0.8134089278	1.2472498684	0.7467849002
O10	-0.6100159772	-0.1697578057	0.9760450364
O11	-1.3446450953	3.7418432082	4.8410257328

2

Gas Phase Energy = -666.341835 hartrees

Zero Point Energy = 63.745 kcal/mol

Vibrational Frequencies(cm^{-1}) : 4.10 5.06 20.83 28.73 54.41 65.40 91.42
91.88 126.65 127.66 129.74 138.01 138.19 139.77 148.58 149.34 209.10
240.44 277.03 280.76 281.53 370.16 370.71 391.93 409.11 409.58 426.18
448.08 569.90 581.57 582.50 593.53 716.20 730.62 745.77 746.21 926.13
931.89 953.57 1034.22 1075.19 1197.91 1328.35 1426.18 1459.51 1492.01
1507.88 1728.56 3015.59 3066.75 3106.26 3136.27 3145.90 3226.60

Coordinates:

C1	-5.8525680980	0.7061757013	0.1408214258
C2	-4.8409288925	0.1716147329	-0.5458982076
C3	-3.9900477237	-0.9771710085	-0.0919296512
H4	-6.4321895664	1.5396550606	-0.2465105909
H5	-6.1383213449	0.3268044576	1.1199181861
H6	-4.5906188491	0.5920503776	-1.5211727807
H7	-4.2949402848	-1.3365816323	0.8965347048
H8	-4.0615276470	-1.8182316359	-0.7949571401
O9	-0.7016600306	-0.5824511664	-0.2034192562
Bi10	1.1558030441	-0.3724762475	-0.2062707019
O11	1.8956701989	1.3846083205	-0.8068930374
Bi12	3.8616935225	1.9260439233	-0.9449242657
O13	4.3956599986	1.3011474614	0.9003517646
Bi14	4.1321878519	-0.4540769581	1.8682526619
O15	2.1224175697	-0.5960565805	1.5299891481
O16	4.6986312597	-1.6685372406	0.3555479719
Bi17	4.2312436652	-1.6888948365	-1.6115721265
O18	2.2056289845	-1.6249252949	-1.3573297510
O19	4.4761212148	0.2867235549	-1.9564824886
H20	-2.9274983312	-0.7010452005	-0.0506657483

TS1 (closed shell)

Gas Phase Energy = -666.318546 hartrees

Zero Point Energy = 60.217 kcal/mol

Imaginary vibrational frequency = 665i cm⁻¹

Vibrational Frequencies (cm⁻¹): -664.81 10.08 12.34 16.64 65.18 88.33 93.53
113.00 123.02 133.92 134.32 139.19 143.46 145.02 168.83 202.42 225.57
257.80 272.62 277.46 280.07 365.90 371.28 381.52 393.14 393.63 407.48
436.67 437.95 535.30 556.00 561.20 587.59 651.25 701.11 730.52 736.58
892.62 932.98 968.56 1004.24 1055.42 1089.36 1216.93 1325.63 1444.41
1505.76 1647.26 1943.31 3142.35 3157.90 3164.33 3239.81 3251.90

Coordinates:

C1	-4.4091795178	1.1434159239	.1412179512
C2	-4.0378032181	.0983318172	-.6275551363
C3	-3.4877123279	-1.1394881774	-.1158620345
H4	-4.8115020600	2.0531821830	-.2923824205
H5	-4.3285414414	1.1074146180	1.2246524383
H6	-4.1252100396	.1854395822	-1.7097206652
H7	-3.5754710958	-1.3169827513	.9546437979
H8	-3.6002477563	-2.0317549441	-.7237274057
O9	-1.1341006179	-1.4144906479	-.2904116167
Bi10	.9076289192	-1.0736710992	-.3178165338
O11	1.1488212535	.8802815323	-.7744608937
Bi12	2.8379170092	2.0037724834	-.7923309661
O13	3.5154753487	1.4823208892	1.0452347653
Bi14	3.7364800043	-.3468227288	1.8881027890
O15	1.8748763346	-1.0448401861	1.4733862979
O16	4.6944514444	-1.2386611982	.3416115488
Bi17	4.3167236373	-1.2598185944	-1.6505308622
O18	2.3738525635	-1.8379687260	-1.5430619358
O19	3.9841595516	.7272868165	-1.8682860162
H20	-2.1084207107	-.9143521323	-.2190493328

3 (Allyl radical)

Gas Phase Energy = -117.265580 hartees

Zero Point Energy = 41.548 kcal/mol

Vibrational Frequencies (cm^{-1}): 426.56 535.24 553.44 778.13 802.29 937.87
1015.80 1042.59 1217.21 1277.70 1429.56 1526.69 1533.86 3147.38 3157.67
3164.07 3257.33 3259.85

Coordinates:

C1	0.4003901406	-0.1685054325	0.0000000000
C2	0.2892145265	1.2103417847	0.0000000000
H3	1.1634475757	1.8512759179	0.0000000000
H4	-0.6828958180	1.6944050384	0.0000000000
C5	-0.6632745781	-1.0529295684	0.0000000000
H6	-1.6889551220	-0.6962322907	0.0000000000
H7	-0.5102194582	-2.1260697890	0.0000000000
H8	1.4051149647	-0.5912938526	0.0000000000

3 ($\text{Bi}_4\text{O}_7\text{H}$)

Gas Phase Energy = -549.066767 h

Zero Point Energy = 22.812 kcal/mol

Vibrational Frequencies (cm^{-1}): 48.75 76.74 91.07 119.39 133.02 135.72 142.31
147.85 151.46 168.35 276.47 297.67 299.70 332.38 374.53 443.70 452.02
464.69 467.41 490.01 514.82 605.37 617.27 643.85 696.77 737.60 759.70
943.27 1114.05 4211.52

Coordinates:

Bi1	-2.0640855463	3.2264995996	-0.3340419215
O2	-0.1843213321	2.4917256017	-0.4579877943
O3	-1.9673602380	3.9278348096	1.5775692460
O4	-2.9928336666	1.4798796589	0.0986448935
Bi5	-2.5663359783	-0.0633103894	1.3382344783
O6	-2.4086156446	1.0375298323	3.0467746664
Bi7	-1.4368355674	2.8397521097	3.2411659530
O8	0.3369938801	2.1971351197	2.5093793595
Bi9	0.8200167362	1.2483094834	0.7881421580
O10	-0.5947776950	-0.1979051437	0.9097996505
O11	-0.2828144333	3.5117295455	4.9211455885
H12	0.5959953311	3.2191065379	4.6097280536

Propene activation on Mo₃O₉

4 (Mo₃O₉)

Gas Phase Energy = -879.929299

Zero Point Energy = 19.578

Vibrational Frequencies (cm⁻¹): 38.34 40.27 49.14 138.52 139.77 172.02 172.09
183.97 184.81 185.67 201.65 249.74 292.27 292.78 298.01 349.64 350.93
359.41 497.56 527.55 528.81 622.77 841.80 842.51 1012.20 1012.74 1020.68
1025.85 1026.24 1037.08

Coordinates:

Mo1	-2.7715344236	0.7146064886	0.9427029781
O2	-0.9923964419	0.7937090910	1.6400579775
O3	-3.4753434077	2.2639361157	0.9338472530
O4	-3.6909156518	-0.4295516919	2.1689667744
O5	-2.8125281503	0.1161653957	-0.6478620576
Mo6	-3.4532891602	-0.7350655905	4.0420428647
O7	-1.5811051949	-0.4549479899	4.3147324422
Mo8	-0.3208600847	0.6772494789	3.4271532763
O9	-4.3593847582	0.3856357133	4.9467646959
O10	-3.9442890987	-2.2951048461	4.5057236173
O11	-0.2903642210	2.2162442408	4.1525032921
O12	1.2570253261	0.0468519014	3.4801729657

5

Gas Phase Energy = -997.851460h

Zero Point Energy = 70.380 kcal/mol

Vibrational Frequencies(cm^{-1}): 23.96 37.37 44.09 45.69 54.69 58.84 69.70
93.21 126.09 129.81 141.33 167.82 171.62 187.51 194.75 195.70 197.88
226.78 262.91 282.40 286.81 296.09 354.80 355.56 361.74 425.97 484.70
518.97 522.48 622.24 630.78 845.64 847.15 926.35 949.87 958.18 1005.55
1006.45 1013.53 1025.36 1026.40 1036.81 1041.59 1076.61 1196.83 1327.69
1416.70 1456.69 1497.97 1501.72 1711.29 3036.77 3087.86 3126.34 3149.16
3156.82 3233.97

Coordinates:

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.9120169285
O3	1.5995022304	0.0000000000	-0.5771129461
O4	-0.8803073684	1.6115584350	-0.5308241539
O5	-0.7562041815	-1.3866415890	-0.6332868942
Mo6	-1.5381789538	3.1323951916	0.4235247344
O7	-1.2659485901	2.7611026932	2.2793600833
Mo8	-0.4328676799	1.3233815622	3.2216085652
O9	-0.6533280942	4.5155462240	-0.0188099018
O10	-3.1708408381	3.4571469664	0.0732805628
O11	0.9890478247	1.8796656605	3.9704409946
O12	-1.4345201282	0.7040496596	4.4498431710
C13	-3.9764692069	0.1703017480	2.1112847998
C14	-3.7319774699	-0.0191635470	0.8084149145
H15	-3.2021162518	-0.8968402958	0.4487242831
H16	-4.1061654384	0.6704880919	0.0552484153
C17	-4.7661784026	1.3090670874	2.6897317882
H18	-5.0625307681	2.0278873711	1.9209339055
H19	-4.1935343274	1.8381837864	3.4608796127
H20	-5.6728482554	0.9331994614	3.1802262008
H21	-3.6104474615	-0.5670941587	2.8270004638

5 - another isomer

Gas Phase Energy = -997.852762 h

Zero Point Energy = 70.983 kcal/mol

Vibrational Frequencies(cm^{-1}): 31.28 38.58 45.12 57.45 82.19 88.40 109.75
134.36 142.33 158.70 171.84 176.35 184.45 194.03 206.66 212.20 219.97
269.56 279.21 286.82 294.70 310.00 342.45 349.33 353.55 423.86 454.94
464.04 533.81 635.90 675.03 837.54 854.82 922.89 955.19 985.66 998.86
1004.42 1010.71 1014.77 1019.79 1026.89 1029.57 1082.72 1204.82 1330.99
1412.69 1456.34 1494.06 1505.70 1665.42 3046.30 3101.16 3145.47 3174.51
3175.60 3269.23

Coordinates:

Mo1	-2.5784534122	0.9807528010	0.8717667687
O2	-0.8503845766	0.9977175817	1.6806163271
O3	-3.2477278530	2.5476876260	0.8238900571
O4	-3.5832071410	-0.1468108670	2.0197422510
O5	-2.5328151075	0.3874754766	-0.7244101285
Mo6	-3.6963115909	-0.7581810728	3.8376077536
O7	-1.7764260911	-0.4369840601	4.1553178842
Mo8	-0.3543084575	0.6009479864	3.4884997721
O9	-4.9149470211	0.2148291996	4.5292955977
O10	-4.2773590718	-2.3579941084	3.7081332264
O11	-0.1933079403	2.0286317137	4.4109738939
O12	1.1211818529	-0.2501928046	3.5753422643
C13	-3.3377256825	-2.3201755998	6.3604542736
C14	-3.2913456965	-0.9939304787	6.6249254072
H15	-4.1869373089	-0.4456092023	6.8956577466
H16	-2.3462757121	-0.4624448086	6.6795129005
C17	-2.1569048538	-3.2044024996	6.1106458676
H18	-1.2292930389	-2.6360421404	6.0129802727
H19	-2.3095136938	-3.8072937200	5.2090389068
H20	-2.0505192950	-3.9085408055	6.9456152176
H21	-4.3103631760	-2.8106868409	6.3638431576

TS2

Gas Phase Energy = -997.799647 h

Zero Point Energy = 66.208 kcal/mol

Imaginary vibrational frequency = 1699i cm^{-1}

Vibrational Frequencies(cm^{-1}): -1698.97 39.86 53.97 58.72 62.59 71.88 82.54
108.61 122.34 138.98 161.84 176.80 182.38 192.38 193.60 205.42 231.95
258.71 278.72 292.84 298.20 306.28 340.46 347.01 411.82 447.91 468.63
476.99 538.33 614.47 636.54 642.47 772.08 818.27 877.42 942.83 954.89
981.37 993.42 998.45 1017.18 1020.16 1023.11 1028.36 1040.26 1173.61
1197.90 1251.84 1306.39 1435.46 1508.74 1590.20 3112.94 3169.73 3177.86
3204.40 3272.71

Coordinates:

C1	1.6677148197	2.0599829406	2.0698527342
C2	0.2768361886	2.0520664711	1.7356136350
C3	-0.2144250279	2.2349466569	0.4733651182
H4	2.3618797128	2.4667979819	1.3332627466
H5	1.9408428743	2.2456139633	3.1084561835
H6	-0.4345502250	1.8385935361	2.5321349001
H7	0.4369047610	2.4478043189	-0.3691575150
H8	-1.2801484591	2.1923603234	0.2772740115
O9	2.3443422904	-0.4312810278	1.9478868864
Mo10	1.4678047427	-1.8436760235	1.2426054040
O11	2.2174784499	-3.3386457202	1.5255381145
O12	-0.3711428349	-1.9030143032	1.8322378904
Mo13	-2.1077051684	-1.4987625103	1.2064874370
O14	-2.5574596723	0.0667601753	1.7354091206
O15	-1.9638051649	-1.5247850697	-0.7027660263
Mo16	-0.4033988382	-1.1766775271	-1.7571990949
O17	-0.3917110441	-2.1009106842	-3.1893867139
O18	1.0529083411	-1.6035748091	-0.6287478818
O19	-0.3404171629	0.4807864671	-2.1781417125
O20	-3.2632276598	-2.6182210660	1.7701457814
H21	2.0285384357	0.7078067636	2.0084012372

6 (open shell singlet)

Gas Phase Energy = -997.808831h

Zero Point Energy = 68.432

Vibrational Frequencies(cm^{-1}): 22.18 48.76 53.10 55.78 64.22 74.33 86.67
114.89 122.73 140.22 144.89 166.80 180.70 182.36 191.06 193.50 203.04
236.58 273.47 278.83 289.86 312.57 341.05 345.84 424.16 444.87 451.61
536.85 580.76 604.61 644.73 724.64 747.87 788.47 813.14 827.35 860.84
876.60 937.61 995.86 1003.00 1017.50 1023.36 1032.42 1033.95 1044.88
1228.29 1274.77 1428.55 1525.27 1530.89 3157.76 3163.85 3176.90 3250.54
3275.38 3318.34

Coordinates:

C1	1.6398427406	2.3981620573	2.1364426351
C2	0.3148120208	2.1372017846	1.7964253161
C3	-0.1869621239	2.1586437367	0.5030586508
H4	2.3605420598	2.7010067640	1.3803873290
H5	1.9538226212	2.4550457046	3.1743429633
H6	-0.3815017383	1.8965446371	2.5990424940
H7	0.4438167991	2.3952625632	-0.3487987357
H8	-1.2362931479	1.9671861152	0.3105725577
O9	2.4369990316	-0.5086992640	2.0091861725
Mo10	1.4671313844	-1.8977512442	1.2243412138
O11	2.0950600308	-3.4603469721	1.3948188648
O12	-0.3756010999	-1.8886353981	1.7959490242
Mo13	-2.1211673465	-1.4948120409	1.1880875844
O14	-2.5965469508	0.0416574738	1.7736087575
O15	-1.9883556552	-1.4664192841	-0.7205558221
Mo16	-0.4192593664	-1.1953983567	-1.7860421485
O17	-0.4025444570	-2.2214386622	-3.1473853227
O18	1.0284916886	-1.5563501244	-0.6240042606
O19	-0.3322162525	0.4223656578	-2.3309871213
O20	-3.2492121650	-2.6536320231	1.7279024655
H21	2.1387996664	0.4377986306	2.0336652140

7 (open shell singlet)

Gas Phase Energy = -997.830688h

Zero Point Energy = 70.552 kcal/mol

Vibrational Frequencies(cm^{-1}): 8.17 24.64 37.96 47.23 67.57 78.83 93.15
96.06 112.78 129.00 150.95 164.51 177.91 183.67 213.34 228.68 256.91
274.91 296.91 309.25 329.75 334.07 369.49 375.61 410.14 425.81 490.49
494.67 588.17 639.50 657.93 709.27 717.38 779.42 800.12 932.69 970.62
976.94 1003.77 1006.64 1011.25 1018.17 1029.36 1036.49 1170.26 1261.51
1322.09 1373.81 1465.20 1506.56 1725.59 3016.58 3097.03 3152.23 3159.93
3243.28 3806.09

Coordinates:

Mo1	-0.1036735869	-0.1899689320	-0.2545972665
O2	-0.3018561608	0.1404457046	1.6124010391
O3	1.5560401455	-0.2803544601	-0.6561924468
O4	-0.9582407400	-1.8411133670	-0.6440165296
O5	-0.8199170676	1.0751689494	-1.1548334392
Mo6	-1.2361674588	-3.4479942443	0.4070905878
O7	-1.0538687160	-2.5186096842	2.0602699943
Mo8	-0.5385435039	-1.0353727131	3.1246363871
O9	0.0530653809	-4.5372608923	0.2499144143
O10	-2.9761236550	-4.1222626694	0.1837754512
C11	-4.7136960711	-4.0212252207	1.8624719234
C12	-4.2997515120	-3.6264131286	0.4749753389
C15	-5.7793196938	-4.7741199635	2.1345737857
H18	-4.0837850955	-3.6474108021	2.6695331734
H13	-4.3057187609	-2.5335465248	0.3534125813
H14	-4.9697942693	-4.0587681587	-0.2750364014
H16	-6.4181533011	-5.1664878696	1.3467814359
H17	-6.0553198519	-5.0215380718	3.1553891344
O19	0.9506863882	-1.3858485078	3.8516828324
O20	-1.9622801957	-0.4290971583	4.2253919858
H21	-2.8678799273	-0.2663144613	3.9209848654

Allyl Oxidation on Mo₃O₉

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Gas Phase Energy = -997.203766h

Zero Point Energy = 61.885 kcal/mol

Vibrational Frequencies(cm⁻¹): 19.39 29.84 34.45 51.99 53.10 62.71 75.75
84.13 122.44 133.20 139.37 160.13 167.51 180.14 190.40 198.52 206.41
251.64 282.82 292.30 303.74 343.33 356.84 367.03 427.62 491.54 526.59
534.31 549.55 583.16 619.43 811.63 834.36 840.97 845.94 939.92 1005.56
1007.64 1015.76 1017.56 1022.91 1024.37 1036.65 1041.70 1219.75 1275.99
1429.98 1528.35 1532.66 3159.46 3161.00 3167.38 3262.98 3267.32

Coordinates:

Mo1	-0.0508080782	0.0135744516	-0.0616967011
O2	0.3412366872	0.1654452049	1.8033302154
O3	1.3151208717	-0.4972057674	-0.9399307971
O4	-0.6650064209	1.7379057787	-0.6155719720
O5	-1.2698654013	-1.1459081055	-0.3119506215
Mo6	-0.9216643664	3.4058298076	0.2851827290
O7	-0.3137389976	3.1285561323	2.0759993121
Mo8	-0.1440799938	1.5059477677	3.0788909695
O9	-0.0865266803	4.6902023645	-0.4581687431
O10	-2.5746074313	3.8079822795	0.2827106936
O11	0.9349465330	1.6206201259	4.3886463025
O12	-1.6750163338	1.1076796374	3.7094586113
C13	3.1580299255	2.0514044129	1.0409917845
C14	3.1604220103	2.6942341164	2.2717217808
H15	3.4931170422	2.1942563873	3.1741567710
H16	2.8598266991	3.7346825118	2.3608310741
C17	2.7761730736	2.6389703397	-0.1582821896
H18	2.4793129440	3.6832791515	-0.2050100915
H19	2.8217310932	2.0898184220	-1.0924670804
H20	3.4815425520	1.0114248604	1.0119862451

9 – another isomer

Gas Phase Energy = -997.204275h

Zero Point Energy = 62.586 kcal/mol

Vibrational Frequencies(cm^{-1}): 26.84 45.07 47.66 56.40 65.36 74.82 90.72
122.47 135.83 154.08 169.52 176.40 187.18 192.97 203.51 210.41 219.56
254.30 278.11 287.60 303.48 342.84 347.99 352.86 426.68 462.70 466.82
530.71 562.40 633.76 671.06 834.68 847.10 895.74 912.52 945.84 1000.90
1005.11 1011.32 1013.46 1018.13 1019.59 1028.66 1045.55 1243.34 1284.99
1432.89 1526.45 1549.46 3170.58 3173.85 3179.41 3268.88 3270.76

Coordinates:

Mo1	-2.6574679714	0.8138118891	0.7982034568
O2	-0.9007639714	1.0148227066	1.5180358007
O3	-3.4334612389	2.3256330133	0.6629249183
O4	-3.5458196553	-0.2832081256	2.0669980743
O5	-2.6354087895	0.1038392585	-0.7499094901
Mo6	-3.5011387763	-0.7112314306	3.9426497608
O7	-1.6359378040	-0.1647076934	4.1848877148
Mo8	-0.2810279563	0.8244950388	3.3203692143
O9	-4.7074575413	0.2292523688	4.6968252012
O10	-3.9141281043	-2.3614858033	4.0686975509
O11	-0.0879943889	2.3451931045	4.0697583080
O12	1.2182307737	0.0151790771	3.3890688852
C13	-4.0151581171	-1.5169069527	7.2099069919
C14	-2.7680121915	-1.2190206026	6.6532916972
H15	-2.3527326658	-0.2201362349	6.7261416544
H16	-2.0909261419	-2.0157377550	6.3582586461
C17	-4.5288247463	-2.7949048448	7.3091954170
H18	-3.9775606402	-3.6519385818	6.9341534737
H19	-5.5010695089	-2.9794880323	7.7529611794
H20	-4.6206906211	-0.6870705393	7.5683235794

TS3

Gas Phase Energy = - 997.199487h

Zero Point Energy = 62.547 kcal/mol

Imaginary vibration frequency = 169i cm⁻¹

Vibrational Frequencies: -169.44 34.58 40.94 53.14 67.78 75.19 83.80
127.54 136.69 147.42 164.17 177.56 184.82 186.80 194.31 209.38 233.15
259.03 283.44 294.09 298.78 316.03 334.51 345.91 428.10 470.02 487.08
534.24 596.73 638.82 694.63 724.64 799.33 833.82 945.08 973.95 982.13
988.20 996.85 1015.45 1017.04 1025.81 1029.80 1049.52 1256.20 1306.26
1443.09 1532.80 1588.64 3180.49 3190.93 3194.25 3282.25 3296.87

Coordinates:

Mo1	-3.2991840874	0.3364198784	1.0490727235
O2	-2.3548976229	1.8265276981	1.7914578555
O3	-4.4821123713	0.8261645071	-0.0755978205
O4	-4.0523586089	-0.5652037419	2.5259564479
O5	-2.1891633457	-0.7020100056	0.2557806651
Mo6	-3.5166322055	-0.8736919428	4.3683052389
O7	-2.4758359827	0.7439927740	4.5758604741
Mo8	-1.4865728469	1.9337627019	3.4977512151
O9	-4.8491599797	-0.9154949382	5.4283452282
O10	-2.5328771930	-2.3036771548	4.4985288853
C11	-0.2407064052	-2.2748204143	2.5056693296
C12	-0.6386142282	-3.1220271915	3.5489945329
H13	-1.2722392852	-3.9802500939	3.3665726270
H14	-0.1665013269	-3.0584423612	4.5234681841
C15	0.7217027455	-1.3122266399	2.6683053739
H16	1.2274798656	-1.1672004547	3.6179632267
H17	1.0296418634	-0.6745055366	1.8479009253
H18	-0.7186347842	-2.3807752515	1.5347132194
O19	-1.4844405058	3.5180354138	4.1281329943
O20	0.1322864611	1.3841846812	3.3440902564

10

Gas Phase Energy = -997.233878h

Zero Point Energy = 64.394 kcal/mol

Vibrational Frequencies: 16.70 19.84 29.10 41.73 50.03 76.11 91.61 124.45
132.93 143.12 162.04 177.00 189.87 193.16 203.24 229.62 263.12 274.61
290.36 301.85 339.22 342.29 377.99 413.53 451.63 476.19 545.30 581.19
634.97 714.81 787.20 823.09 935.97 963.12 983.86 987.45 999.62 1010.44
1013.95 1020.90 1034.05 1038.92 1167.43 1259.06 1334.98 1374.85 1462.83
1505.46 1720.84 3049.97 3115.92 3155.12 3166.33 3245.46

Coordinates:

Mo1	-2.7089674953	1.1940196266	0.9344780460
O2	-1.4502026059	2.0079646430	2.1289584179
O3	-4.1622370314	2.0863180482	0.8949140668
O4	-2.9795309304	-0.5379896438	1.6580537168
O5	-2.0982401960	1.0891186707	-0.6549709108
Mo6	-3.0378857450	-1.4445037099	3.3673852442
O7	-2.0165852552	-0.0524874605	4.2503185858
Mo8	-0.7323694113	1.2242829880	3.7180547130
O9	-4.5986772007	-1.4603965798	4.0223119291
O10	-2.1501644850	-3.0770054205	3.2937969677
C11	0.2476227564	-3.1011999078	3.7676713194
C12	-0.8647073336	-3.6512397254	2.9261473918
H13	-0.7127609752	-3.4372600243	1.8612697840
H14	-0.9731676566	-4.7310099940	3.0609663186
C15	0.8794473546	-3.8244229315	4.6932605667
H16	0.6136092477	-4.8602633579	4.8913831356
H17	1.6925713944	-3.4076307805	5.2799454726
H18	0.5402760111	-2.0684121439	3.5813833295
O19	-0.4340467162	2.3721421560	4.9427503372
O20	0.7297034598	0.4051746512	3.3584300

10 (another conformer)

Gas Phase Energy = -997.237075h

Zero Point Energy = 64.885kcal/mol

Vibrational Frequencies: 50.18 51.68 61.36 66.66 83.83 91.91 120.09
122.89 141.93 159.57 175.31 184.16 195.44 199.83 213.73 245.91 256.52
274.70 291.72 302.30 341.10 347.14 384.08 436.83 448.87 460.02 535.44
616.06 646.80 703.86 801.85 827.94 926.08 967.94 985.57 996.65 1003.72
1006.99 1019.13 1024.44 1033.34 1035.13 1165.21 1256.67 1320.05 1372.25
1460.47 1497.63 1713.42 3059.80 3108.96 3170.13 3171.07 3253.64

Coordinates

Mo1	-2.4325148799	0.1793284796	0.7255165474
O2	-1.5049563726	1.6225919963	1.5736623761
O3	-3.6952556150	0.7466828762	-0.2690437248
O4	-3.0916787373	-0.8866258744	2.1416749922
O5	-1.3622313534	-0.7432103393	-0.2390393408
Mo6	-2.7836400741	-1.2439221726	4.0186463562
O7	-1.7433758892	0.3583997094	4.3050961107
Mo8	-0.8242806676	1.7152115915	3.3599615699
O9	-4.2334877904	-1.1241209917	4.8843036508
O10	-1.7662028400	-2.7810250203	4.3322722102
C11	-0.0954230451	-2.6382249901	2.5437943400
C12	-0.4458462200	-3.1962294400	3.8914056309
H13	-0.4760579217	-4.2914033478	3.8849360762
H14	0.2631600385	-2.8684924027	4.6594288252
C15	0.8894857129	-1.7581892955	2.3406125886
H16	1.5091079138	-1.3859040510	3.1524322807
H17	1.1085137609	-1.3818020149	1.3460651663
H18	-0.6931314839	-2.9912727779	1.7045051992
O19	-1.0888500116	3.2510594079	4.0501728760
O20	0.8563193979	1.3996846388	3.3858357802

TS4

Gas Phase Energy = -997.177174h

Zero Point Energy = 60.881

Vibrational Frequencies: -1069.49 16.21 40.13 57.40 78.15 111.29 129.51
135.02 148.01 157.62 159.90 173.28 196.89 200.00 218.51 234.59 249.94
286.06 302.02 320.85 329.83 342.92 370.94 425.53 461.70 476.95 548.02
568.36 605.15 611.96 679.35 763.06 782.26 861.03 939.52 956.63 999.04
1011.75 1015.64 1019.22 1028.96 1111.99 1157.47 1213.67 1243.90 1307.17
1330.84 1378.34 1475.50 1668.45 3082.58 3164.51 3179.46 3260.05

Coordinates:

Mo1	-0.0402039213	-0.0088519497	0.0728234497
O2	0.2926140116	0.3026749300	1.9190845300
O3	1.3039344426	-0.2002169951	-0.9492205387
O4	-1.0282595137	1.5029786147	-0.3860096553
O5	-1.1839160233	-1.4323866929	-0.0124636615
Mo6	-2.8917149586	1.7681422011	0.1908906331
O7	-2.3478242786	1.8230835895	2.0776454828
Mo8	-1.0759356634	0.9263774032	3.1461621241
O9	-3.5276043483	3.0569464500	-0.7020318171
H10	-2.2941701513	-1.4139463561	-0.1774825497
C11	-4.5335256515	-2.0081303090	-0.8398900503
C12	-3.7540169669	-1.1828012734	0.0635209000
H13	-3.5917336210	-1.5435797625	1.0856618800
C14	-4.7505147953	-3.3223144760	-0.6406984279
H15	-4.3813705833	-3.8352399815	0.2436311187
H16	-5.3019354724	-3.9181885295	-1.3593734054
H17	-4.9075259621	-1.5143586844	-1.7348490869
O18	-0.4380581976	1.9355614398	4.3633324149
O19	-1.8143441211	-0.4283657776	3.8878472599
O20	-3.9033224007	0.1557111286	-0.0216937142

TS4'

Gas Phase Energy = -997.180595 h

Zero Point Energy = 60.068 kcal/mol

Imaginary frequency = 1768i cm⁻¹

Vibrational Frequencies: -1767.52 18.14 33.84 43.35 75.67 105.59 113.59
131.33 153.82 155.51 157.10 171.75 180.69 208.54 221.24 237.02 247.12
273.31 287.76 303.31 311.73 344.56 385.68 444.62 468.36 518.61 534.86
553.64 599.74 619.31 678.94 708.24 793.26 832.34 932.36 968.64 996.93
1007.18 1014.48 1019.56 1023.72 1034.53 1051.15 1110.03 1184.25 1270.26
1311.42 1383.94 1452.94 1632.24 3092.40 3171.94 3178.71 3268.77

Coordinates:

Mo1	0.0119480587	-0.0018196627	-0.0059887164
O2	-0.0507010378	-0.0982892785	1.9116572703
O3	1.5121751575	0.1413243692	-0.7885465427
O4	-1.0637609999	1.4972204268	-0.4093829882
O5	-1.0353940536	-1.3219393183	-0.7188781076
Mo6	-2.9572090465	1.6418765458	-0.1157733561
H7	-2.0457475207	-1.1339658788	-1.2308789897
C8	-3.4108221726	-0.8777334354	-1.6845712316
O9	-3.3352263071	3.2159988982	-0.6079415337
O10	-3.8670521993	0.3000607731	-1.1389073868
C11	-3.3126921654	-0.9637707064	-3.1292872288
Mo12	-1.5302804626	0.4917243065	2.9847335663
H13	-3.7947701849	-1.7513911024	-1.1474718151
O14	-2.8303844658	1.1252340072	1.7483056692
C15	-3.4382370507	0.0705218556	-3.9867947858
H16	-3.6673947313	1.0732995217	-3.6408689494
H17	-3.3301817563	-0.0749905990	-5.0557894754
H18	-3.0786416641	-1.9581051020	-3.5056868333
O19	-1.0422930577	1.7250262785	4.0575431664
O20	-2.1673466630	-0.8004174718	3.9014138264

11

Gas Phase Energy = -997.211037h

Zero Point Energy = 63.116 kcal/mol

Vibrational Frequencies: 22.97 47.09 49.55 62.73 87.28 104.83 113.61
125.39 141.10 146.80 157.81 171.52 176.29 181.52 198.39 222.40 237.56
261.81 273.10 296.65 319.23 326.57 338.59 350.79 368.94 412.60 492.06
538.45 616.09 640.26 645.79 672.80 702.54 728.00 753.70 954.41 961.18
984.83 1001.41 1004.67 1019.73 1030.79 1031.82 1210.75 1309.41 1394.64
1461.24 1579.84 1666.81 3096.40 3167.17 3197.68 3263.16 3829.34

Coordinates:

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.9077598073
O3	1.5819668842	0.0000000000	-0.6140405049
O4	-0.6828844006	1.7630889943	-0.3221814552
O5	-1.2989993687	-1.2558344649	-0.6172591237
Mo6	-1.0713695522	3.4897381761	0.3959131029
O7	-0.4981367173	2.9353683169	2.2113800839
Mo8	-0.8376018357	1.3200448689	3.0532065900
O9	-0.1628884363	4.8220272747	-0.1045001818
O10	-2.7978569142	4.1480900783	1.2441556321
C11	-4.6288483928	4.7616384515	2.5886890972
C12	-3.6982317513	3.8000782179	2.0567974241
H13	-3.7656878212	2.7497520036	2.3639215996
C14	-5.5654138474	4.3926360918	3.4842110403
H15	-5.6545892682	3.3619347824	3.8175971467
H16	-6.2563807741	5.1104757959	3.9133256645
H17	-4.5253552171	5.7910409776	2.2550064951
O18	-0.2300290918	1.2926826356	4.6540267528
O19	-2.5455512716	1.0281922268	3.0227990156
H20	-1.0536386298	-2.0218471746	-1.1563456684

12 (Mo₃O₈H)

Gas Phase Energy = -805.246141h

Zero Point Energy = 22.962 kcal/mol

Vibrational Frequencies: 33.02 49.49 62.15 111.85 115.10 127.25 138.29
157.62 170.18 175.22 220.70 239.59 260.08 277.94 295.20 334.50 385.45
432.33 455.99 552.68 623.52 659.81 726.16 757.28 798.88 1004.49 1013.98
1026.10 1037.50 3819.80

Coordinates:

O1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	2.9972603832
O3	2.7458214412	0.0000000000	1.4739126767
Mo4	-0.2760111837	3.5782721000	0.3307104270
O5	-0.9041658148	2.6551945240	-1.2372418112
Mo6	-1.2084925911	0.7689647513	-1.2606257522
O7	-1.1726674021	4.8279405410	1.0291546775
O8	0.6753469120	2.3383347792	1.4261694722
Mo9	0.9063371410	0.4439855714	1.6363425996
O10	-2.8236838294	0.4281364639	-0.8230887870
O11	-0.9235292025	0.1222416571	-2.8146579526
H12	3.2247480872	-0.5377245391	2.1222510512

12 – quartet

Gas Phase Energy = -805.253755h

Zero Point Energy = 22.965 kcal/mol

Vibrational Frequencies: 42.02 50.62 58.16 109.09 112.45 123.41 127.69
157.22 169.34 182.41 217.70 238.38 264.70 265.29 292.83 334.37 385.83
445.35 465.28 526.47 617.35 660.43 726.48 793.78 813.03 1002.73 1010.82
1019.46 1028.66 3822.84

Coordinates:

O1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	2.9504405092
O3	2.7706769209	0.0000000000	1.4399457412
Mo4	-0.3836033023	3.5503309950	0.4195124296
O5	-1.3074714650	2.5254140114	-0.9481764366
Mo6	-1.4161411016	0.6324913304	-1.0975928874
O7	-0.5622761992	5.2004252991	0.7604556789
O8	0.7537226697	2.3675832459	1.4375730514
Mo9	0.9383741867	0.4679062109	1.6167540219
O10	-2.9214390485	0.0777009242	-0.5060912835
O11	-1.2347059025	0.1074182521	-2.7130479419
H12	3.2507374780	-0.5452640604	2.0807563033

12 – another isomer

Gas Phase Energy = -805.251060h

Zero Point Energy = 24.014 kcal/mol

Vibrational Frequencies: 85.02 92.27 114.64 126.40 133.89 149.12 163.07
172.91 182.32 224.63 235.94 279.31 280.99 312.02 334.83 347.83 449.73
502.36 524.88 573.35 599.11 682.62 720.13 741.27 979.88 1000.98 1018.13
1022.61 1037.24 3710.82

Coordinates:

O1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	3.3075874647
O3	2.7496221278	0.0000000000	1.2762739306
Mo4	3.0716011242	1.8318962970	0.4072342559
O5	2.3203561509	1.4212530283	-1.3201872672
Mo6	1.1570303089	-0.1144871687	-1.4825357913
O7	4.5968195514	2.5192561977	0.6984214290
O8	1.6708283550	2.1629991571	1.5972817857
Mo9	0.6725534989	0.4295919934	1.8197821203
O10	0.3235370649	-0.1856024022	-2.9682784364
O11	2.1475776220	-1.5107034940	-1.2881363661
H12	2.9898182635	-0.8087189084	0.7872001407

12 (Acrolein)

Gas Phase Energy = -191.914050h

Zero Point Energy = 38.589 kcal/mol

Vibrational Frequencies: 178.43 318.61 571.47 611.61 925.61 994.01 1024.06
1042.93 1173.96 1300.08 1400.47 1464.09 1696.09 1805.08 2890.39 3154.31
3193.77 3248.08

Coordinates:

C1	0.6078563787	0.4804666203	0.0000000000
C2	0.4106001201	1.8032782743	0.0000000000
H3	1.2319845355	2.5123842010	0.0000000000
H4	-0.5944103657	2.2198179742	0.0000000000
C5	-0.5280273096	-0.4603432901	0.0000000000
H6	-1.5309551060	0.0244145720	0.0000000000
O7	-0.4125719639	-1.6702138945	0.0000000000
H8	1.6017410634	0.0399592804	0.0000000000

O₂

Gas Phase Energy = -150.316606h

Zero Point Energy = 2.375 kcal/mol

Vibrational Frequencies: 1661.34

Coordinates:

O1	0.0000000000	0.0000000000	-0.6070774288
O2	0.0000000000	0.0000000000	0.6070774288

13

Gas Phase Energy = -1147.578850h

Zero Point Energy = 66.607 kcal/mol

Vibrational Frequencies: 14.50 29.10 31.34 43.90 49.27 84.14 106.57 110.69
124.99 129.14 138.60 153.55 155.17 163.13 169.90 180.13 198.85 209.48
219.64 228.07 248.42 275.31 286.69 297.75 299.19 338.96 345.90 369.73
383.60 398.30 454.06 486.66 525.81 613.67 621.55 626.62 667.34 724.19
743.95 800.61 952.12 998.60 1006.55 1016.76 1019.38 1026.89 1030.14
1063.43 1140.78 1211.01 1308.85 1393.80 1470.98 1681.71 1714.67 3059.73
3165.10 3208.76 3260.97 3827.80

Coordinates:

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.9165513037
O3	1.5965731987	0.0000000000	-0.5748886200
O4	-0.6689270430	1.7316291886	-0.2111282088
O5	-1.2648460008	-1.2652109311	-0.6425968525
Mo6	-1.0585543372	3.5236907170	0.3736656388
O7	-0.7872210753	2.9726603977	2.2668813149
Mo8	-0.7775844514	1.2968754409	3.1052824925
O9	0.3022223061	4.4113169011	-0.1086749032
O10	-1.8205288363	5.4481448413	1.2904132436
C11	-2.0112979370	7.1017253754	2.9586703367
C12	-1.5475115779	5.8282560457	2.4364231110
H13	-0.9371571235	5.1856966807	3.0891586113
C14	-1.6635320216	7.4814408293	4.1985007793
H15	-1.0423234448	6.8504266357	4.8296706034
H16	-1.9845508805	8.4292632900	4.6183151097
H17	-2.6288437250	7.7139297424	2.3075196305
O18	0.1042111699	1.3926039692	4.5690739816
O19	-2.3826890378	0.8247051030	3.4742836529
H20	-1.0263262396	-1.9938087581	-1.2344903947
O21	-2.7035225691	3.6753284852	-0.7302170432
O22	-3.2882292950	3.3132736373	0.4152378583

13 – quartet

Gas Phase Energy = -1147.567981h

Zero Point Energy = 66.695 kcal/mol

Vibrational Frequencies: 10.60 22.55 29.20 40.05 47.52 78.56 100.23
106.92 116.12 123.34 131.93 140.49 146.64 152.73 166.53 171.46 188.65
200.68 222.10 226.72 255.58 271.29 282.34 288.99 309.12 329.87 356.60
363.31 379.32 443.39 455.26 493.38 517.50 613.48 626.59 642.71 660.16
720.76 772.69 815.13 951.49 1000.07 1006.15 1013.90 1019.39 1025.74
1030.03 1063.35 1210.10 1215.86 1308.82 1394.83 1471.29 1682.31 1719.38
3052.58 3164.95 3208.70 3261.11 3833.10

Coordinates:

Mo1	0.0000000000	0.0000000000	0.0000000000
O2	0.0000000000	0.0000000000	1.9313234219
O3	1.6286653893	0.0000000000	-0.4770553978
O4	-0.7447241707	1.7310088548	-0.2807230944
O5	-1.2461849427	-1.2886598447	-0.6420054961
Mo6	-0.6605482343	3.5482929507	0.3815553572
O7	-0.0508108378	2.9932737542	2.1707661596
Mo8	-0.2071123700	1.4103623808	3.1837453404
O9	0.5794144875	4.2782199430	-0.5160319798
O10	-0.8696673748	5.6068227134	1.3672016894
C11	-0.2833813325	7.3175320072	2.8831593493
C12	-0.2310233825	5.9610014861	2.3654257563
H13	0.4053850883	5.2304102151	2.8887508990
C14	0.4685289260	7.6550932738	3.9427505755
H15	1.1126491588	6.9286761944	4.4326413351
H16	0.4680938931	8.6613297561	4.3489257421
H17	-0.9317097249	8.0239997234	2.3725399132
O18	1.0009443445	1.3658205991	4.3966337922
O19	-1.7404628597	1.3189794316	3.9420969463
H20	-1.0100983547	-1.9890925663	-1.2672656321
O21	-2.5626768334	3.7989065965	-0.4394262339
O22	-2.8076093675	3.7715468771	0.8589916015

13'

Gas Phase Energy = -1147.597031h

Zero Point Energy = 68.084 kcal/mol

Vibrational Frequencies: 31.18 41.58 67.83 81.75 102.26 107.47 120.85
133.13 138.98 154.17 161.70 165.77 177.60 183.45 194.52 206.62 229.20
233.43 247.86 250.83 276.11 295.75 297.62 303.16 337.24 349.98 369.51
389.71 429.65 466.09 502.03 538.62 621.95 635.03 647.97 685.44 713.59
791.63 802.62 845.93 887.07 959.76 983.05 1012.47 1014.00 1015.62 1033.19
1035.07 1055.64 1219.02 1312.56 1406.98 1475.45 1648.76 1685.41 3104.55
3169.18 3209.55 3265.21 3802.85

Coordinates:

Mo1	0.0750042705	-0.2544793222	0.1388796831
O2	1.9396239192	-0.4000889914	0.0064907563
O3	-0.3388223600	1.0761237861	-0.8380758186
O4	-0.3819029315	0.2444716883	1.8036374653
O5	-1.0013869210	-1.5764521002	-0.6897266270
Mo6	0.3049926846	-1.0305922550	3.3493818306
O7	2.1683385791	-0.3378164291	3.0313014094
Mo8	3.1350472103	-0.7876573841	1.5160307055
O9	-0.5326352994	-0.2750262898	4.6157976686
O10	1.2706446814	-2.6038941302	4.4126732982
C11	2.5476706584	-4.5650663310	4.6575035757
C12	1.8364330361	-3.5807275635	3.8759170592
H13	1.8063812313	-3.6835385833	2.7840632406
C14	3.2154669182	-5.5471051926	4.0267301818
H15	3.2230728844	-5.6159751582	2.9419720325
H16	3.7804752075	-6.2955680986	4.5728418723
H17	2.5367666057	-4.4599766295	5.7386167979
O18	4.5405189578	0.1739717365	1.4261617468
O19	3.6278396171	-2.4343196538	1.5638172900
H20	-1.5182517838	-1.2873262053	-1.4582353498
O21	0.5401140774	-2.1717100837	1.4703568437
O22	-0.5925025913	-2.4222337775	2.3541821403

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Gas Phase Energy = -955.65765914721

Zero Point Energy = 27.163 kcal/mol

Vibrational Frequencies: 43.45 51.48 59.12 112.45 128.04 132.63 147.71
152.94 158.30 170.31 187.36 192.22 240.93 243.82 253.53 272.59 281.98
300.62 318.17 340.03 370.89 413.01 488.04 598.92 614.37 673.18 735.43
762.60 813.35 857.11 957.56 1005.01 1018.27 1040.82 1045.03 3819.61

Coordinates:

Mo1	-0.0092673417	0.0033985639	0.0647509103
O2	1.8201218060	-0.1176111654	-0.0880183844
O3	-0.5171419819	1.5728121091	-0.3192727125
O4	-0.3847375179	-0.3332490330	1.7758135750
O5	-0.8579927165	-1.2565778129	-1.0370555445
Mo6	0.3985154083	-1.2228552748	3.5235409611
O7	2.1908930100	-0.7711335301	2.7582108624
Mo8	3.1968513683	-0.7631728047	1.2136925340
O9	-0.0063632343	-0.2509508748	4.8416696476
O10	4.5463462768	0.2737164504	1.3289048969
O11	3.7234373861	-2.3299623662	0.7820791941
H12	-1.4402520891	-1.0265139174	-1.7773462581
O13	0.6823024329	-3.0633096899	3.9874909243
O14	-0.6070285349	-2.8564979545	3.3406072871